Principles of Mathematical Modelling

- describe a given problem with some mathematical formalism in order to
  - get a formal and precise description
  - see fundamental properties due to the abstraction
  - allow a systematic treatment and, thus, solution
- (mathematical) model: formal description (and usually simplification) of (some) reality
- bigger or smaller evidence:
  - exact natural science and engineering: long tradition (basic conservation laws of continuum mechanics, e.g.)
  - economics, game theory, climate modelling: many open questions (Keynes or not, MinMax or not, chaos or not?)
- to do: both *derivation* and *analysis* of models

Derivation of a Model 1

- What do you want to model?
  - a catalyst‘s function or the detailed reactions in it?
- Which are the important quantities for that?
  - Example 1: Optimum trajectory of the Space Shuttle – gravitation of Pluto, gravitation of the Earth?
  - Example 2: Prediction of Dow Jones Index tomorow – statements of Mr. Greenspan, statements of myself?
- How important are they?
  - Think of consequences of a neglection!
- What are their relations and interactions?
  - *qualitative* and *quantitative* aspects
- How can these be (mathematically) described?
  - algebraic or differential equations, graphs, automata, ...

Derivation of a Model 2

- description of relations and interactions:
  - position, speed, and acceleration of an oscillating pendulum?
    ordinary differential equation!
  - deformation of a membrane under some load?
    partial differential equation!
  - initial or boundary conditions of some growth process?
    algebraic equations!
  - non-negativity of some quantity?
    algebraic inequality!
  - order of several steps?
    graphs!
  - state transitions?
    automata!

Derivation and Analysis of Models

- Of which type is the resulting task?
  - Is there a solution (Hamiltonian way in a graph)?
  - Find a/the solution (flow field around an aircraft)!
  - Find a/the best solution (shape optimization)!
- What can be said about solution(s) concerning
  - their existence?
  - their uniqueness?
  - their dependency on the input data?

  (*well-posed problems:* Hadamard 1923; Tikhonov, John; cf. *inverse problems*)
- Is the model well-suited for a numerical treatment?
- Is the model derived so far correct?
  - validation (experiments)!

What to do with models?

- the analytical approach:
  - prove existence and uniqueness formally
  - construct or find solution(s) formally/directly/analytically
  - desirable, but almost never possible
- the heuristic approach:
  - trial and error, following some (hopefully smart) strategy
  - useful in discrete problems (travelling salesman etc.)
- the direct numerical approach:
  - follow some numerical algorithm and end up with the exact solution (Simplex algorithm for linear programming)
- the approximative numerical approach:
  - approximate/discretize the model equations and end up with some approximate solution

Classes of Mathematical Models

- Models can be discrete or continuous:
  - discrete models use a discrete/combinatoric description (integer numbers, graphs, ...)
  - continuous models use real quantities (real numbers, physical quantities, differential equations, ...)
  - primarily, but not necessarily: discrete models for discrete phenomena, continuous models for continuous phenomena
  - examples: lattice-gas-automata for fluid flow, continuum mechanics for traffic flow
- Models can be deterministic or stochastic:
  - again no general relation between phenomena and models
  - roll the die: random phenomenon, stochastic model
  - crash test: deterministic phenomenon, deterministic model
  - but what about weather or data traffic through the internet?

Discrete Models 1: Scheduling

- n jobs to be done on m machines working in parallel:
  - no job simultaneously on more than one machine
  - no machine working simultaneously on more than one job
- several model parameters:
  - characterizing the jobs: subjobs, processing time, earliest starting time, due time, weighting, cost of delay, ...
  - characterizing machines and processing: identical or different machines, order of subjobs important or not, precedence relations of jobs
  - criteria of optimality: time of completion, delay, idle times
- task: find the best schedule with respect to some objective function (minimizing overall time, e.g.)
- model: graph with disjunctive and conjunctive edges

Discrete Models 2: Elections

- m candidates, n voters; model: theory of relations
- task: derive a reasonable *collective* preference from the different reasonable *individual* preferences
- possible choices:
  - external dictator: individual preferences do not matter ☹
  - internal dictator: one individual preference always wins ☹
  - majority wins: cycles (a>b>c>a) cannot be excluded ☹
  - something else democratic – but what is democratic?
    - all reasonable individual preferences are allowed
    - the collective preference must be reasonable
    - everything is possible with unanimity
    - no dictator, independence of irrelevant alternatives

    impossible if m>2 and n>1 (Arrows, 1951)!!
- drawback of democracy or drawback of our model??

Discrete Models 3: Event Simulation

- task: model data or job traffic through computer system, optimize flow, find and avoid bottlenecks
- model: discrete event simulation, stochastic processes
  - elementary queueing system (service stations, waiting pool)
  - quantities: waiting time, service time, staying time; filling, capacity, throughput
  - arrival and completion of jobs: stochastic processes (deterministic D, Markovian M, or general G)
  - notation: M|M|1 (arrival and completion neg. exp., 1 station)
  - service strategies: FCFS, LCFS, random, round robin, ...
  - queueing nets: network of elementary queueing systems
- computer systems: discrete space of states, state transitions driven by stochastic processes, Markovian chains or systems, resp.

Hierarchy and Multiscale Property

- often to be chosen: scale/level of observation:
  - Which resolution is necessary (w.r.t. the model's accuracy)?
  - Which resolution can be tackled numerically?
- flow through a cylinder – how many dimensions?
  - 1D: neglect cross-section
  - 2D: exploit symmetries
  - 3D: full resolution
- electric circuit simulation – spatial resolution or not?
  - std. system simulators (SPICE, TITAN): only time, ODEs
  - parasitic cross effects: take space into account!
- turbulence – which vortices can be neglected?
  - significant transport of energy between different scales
  - direct simulation – Large Eddy Simulation – averaging models

Averaging and Homogenization

- often: coarse-grain phenomena are of interest, but fine-grain phenomena must not be neglected
- try to do some averaging:
  - in time: turbulence, molecular dynamics
  - in space: flow and transport through porous media (a catalyst or soil)
- formal concept: homogenization
  - representative elementary volume
  - scaled reproduction, translation, periodic continuation
  - limit process of scaling factor
  - new quantities (effective parameters: porosity, permeability)
  - new equations (porous media: instead of transport equations now Darcy-Forchheimer equation)